

=> fil reg; d stat que l3; d sqide l3 1-2; fil capl uspatf; s l3
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STRUCTURE FILE UPDATES: 4 DEC 2005 HIGHEST RN 869277-23-6
DICTIONARY FILE UPDATES: 4 DEC 2005 HIGHEST RN 869277-23-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

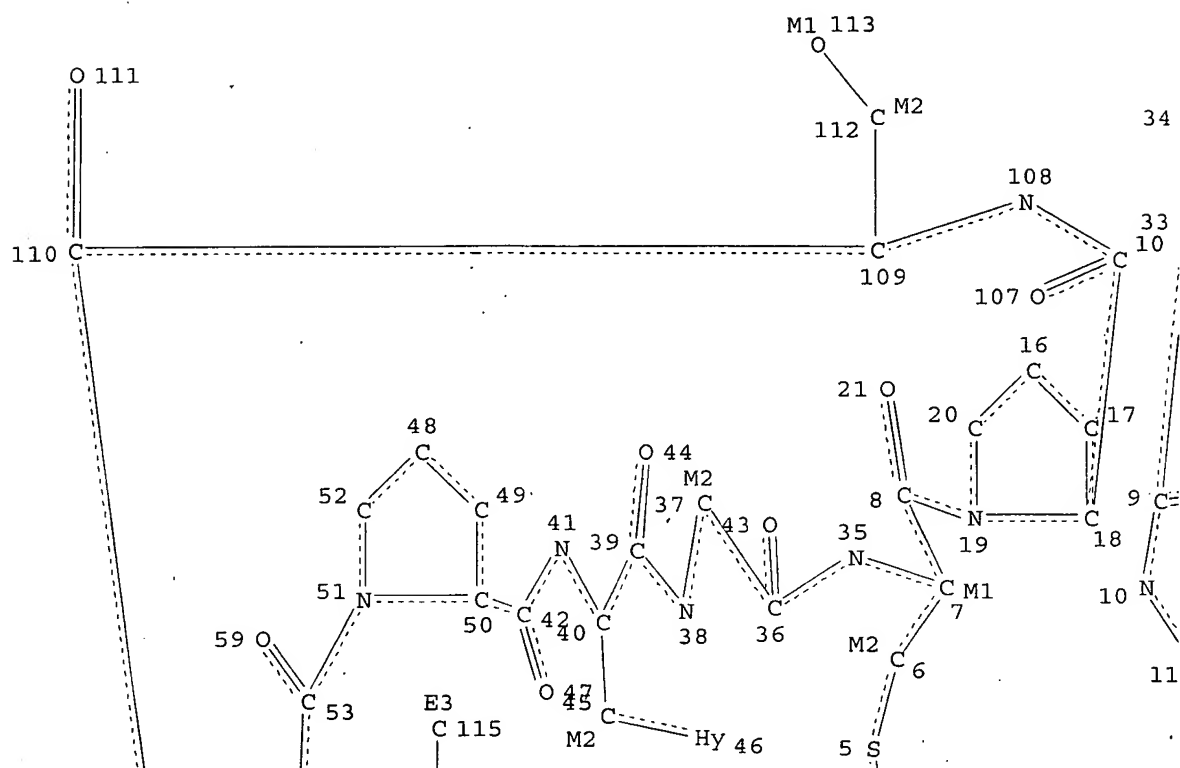
*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

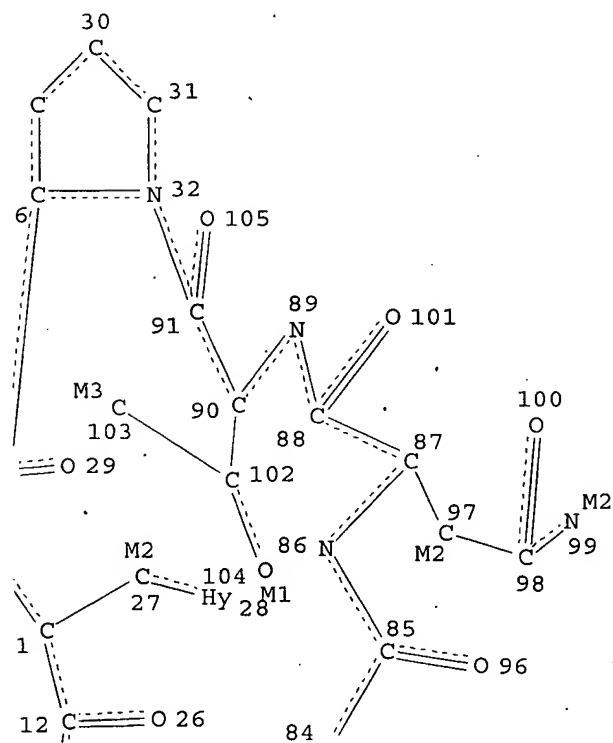
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

L1 STR

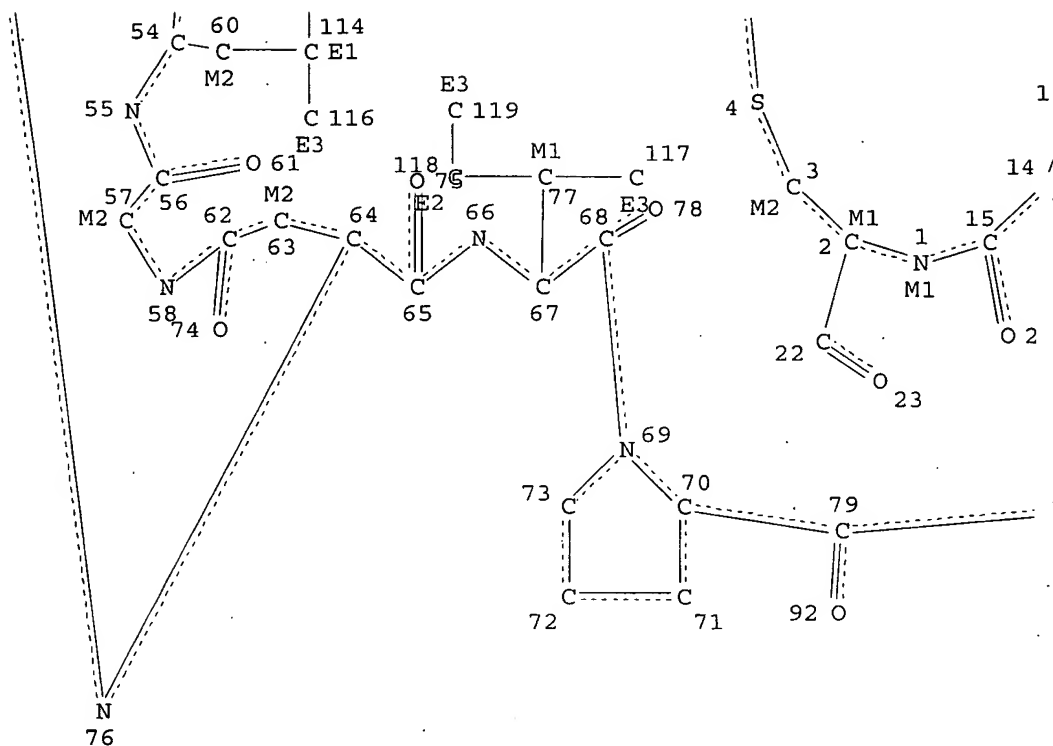


Page 1-A

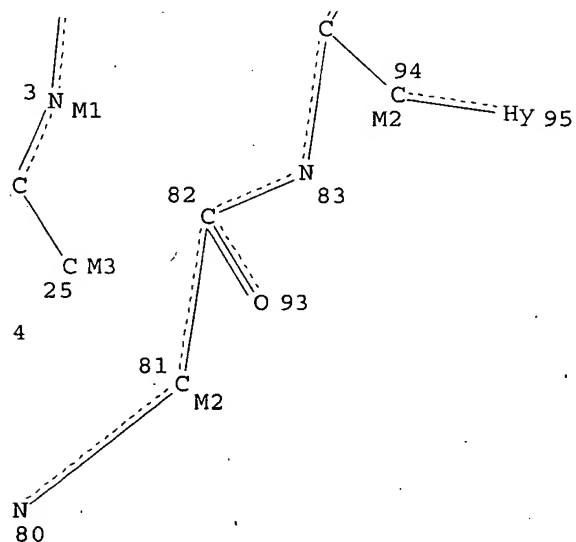


Page 1-B

structure
displayed
in easier-to-view
format at blue tab



Page 2-A



Page 2-B

NODE ATTRIBUTES:

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MLEVEL IS CLASS AT 21 22 23 24 25 26 27 29 43 44 45 47 59 60 61 74 75
77 78 92 93 94 96 97 98 99 100 101 102 103 104 105 107 111 112
113 114 115 116 117 118 119

GGCAT IS PCY HIC LOQ UNS AT 28

GGCAT IS PCY HIC LOQ UNS AT 46

GGCAT IS PCY HIC LOQ UNS AT 95

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 119

STEREO ATTRIBUTES: NONE

L3 2 SEA FILE=REGISTRY SSS FUL L1

100.0% PROCESSED 270 ITERATIONS

2 ANSWERS

SEARCH TIME: 00.00.01

L3 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN

RN 647807-36-1 REGISTRY

CN L-Cysteine, glycyl-L-leucyl-L-prolyl-L-tryptophylglycyl-L-cysteinyl-L-prolyl-L-seryl-L- α -aspartyl-L-isoleucyl-L-prolylglycyl-L-tryptophyl-L-asparaginyl-L-threonyl-L-prolyl-L-tryptophyl-L-alanyl-, 19-methyl ester, (9 \rightarrow 1)-lactam, cyclic (6 \rightarrow 19)-disulfide (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

SQL 19

NTE modified (modifications unspecified)

type	location	description
bridge	Gly-1 - Asp-9	lactam
bridge	Cys-6 - Cys-19	disulfide bridge

SEQ 1 GLPWGCPSDI PGWNTPWAC

RELATED SEQUENCES AVAILABLE WITH SEQLINK

MF C96 H127 N23 O24 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L3 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN
RN 647807-35-0 REGISTRY
CN L-Cysteine, glycyl-L-leucyl-L-prolyl-L-tryptophylglycyl-L-cysteinyll-L-prolyl-L-seryl-L- α -aspartyl-L-isoleucyl-L-prolylglycyl-L-tryptophyl-L-asparaginyll-L-threonyl-L-prolyl-L-tryptophyl-L-alanyl-, (9 \rightarrow 1)-lactam, cyclic (6 \rightarrow 19)-disulfide (9CI) (CA INDEX NAME)

OTHER NAMES:

CN BI 32169
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 19
NTE

type	location	description
bridge	Gly-1 - Asp-9	lactam
bridge	Cys-6 - Cys-19	disulfide bridge

SEQ 1 GLPWGCPSDI PGWNTPWAC

RELATED SEQUENCES AVAILABLE WITH SEQLINK

MF C95 H125 N23 O24 S2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL
DT.CA Caplus document type: Journal; Patent
RL.P Roles from patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PRP (Properties)

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

FILE 'CAPLUS' ENTERED AT 16:55:14 ON 05 DEC 2005
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FILE 'USPATFULL' ENTERED AT 16:55:14 ON 05 DEC 2005
CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS).

L8 4 L3

=> dup rem l8

PROCESSING COMPLETED FOR L8

L9 4 DUP REM L8 (0 DUPLICATES REMOVED)

ANSWERS '1-3' FROM FILE CAPLUS

ANSWER '4' FROM FILE USPATFULL

=> d ibib ed abs hitrn 1-4; fil hom

L9 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:60541 CAPLUS

DOCUMENT NUMBER: 140:105298

TITLE: Bicyclic oligopeptides and their use as glucagon receptor antagonists

INVENTOR(S): Potterat, Olivier; Streicher, Ruediger; Wagner, Klaus; Maurer, Till; Mack, Juergen; Peters, Stefan

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. KG, Germany

SOURCE: PCT Int. Appl., 33 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004007535	A1	20040122	WO 2003-EP7657	20030715
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2489189	AA	20040122	CA 2003-2489189	20030715
EP 1525218	A1	20050427	EP 2003-763864	20030715
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
US 2004072736	A1	20040415	US 2003-621272	20030717
PRIORITY APPLN. INFO.:			EP 2002-15907	A 20020717
			US 2002-416797P	P 20021008
			WO 2003-EP7657	W 20030715

OTHER SOURCE(S): MARPAT 140:105298

ED Entered STN: 26 Jan 2004

AB The invention relates to a bicyclic oligopeptide or ester thereof having the capability to inhibit the glucagon receptor, which essentially consists of (a) a first cyclic group, which comprises at least one cysteine group and is formed by an amide bonding of the N-terminal amino acid with the second carboxylate group of a diacid amino acid, and (b) a second cyclic group which is formed by an amide bonding of an amino acid with the -carboxylate group of said diacid amino acid, and by a disulfide bonding of the C-terminal cysteine and a cysteine group within the first cyclic group (a); and to the use of such bicyclic oligopeptides for the preparation of a medicament for the treatment or prevention of diseases, in which glucagon receptors are involved.

IT 647807-35-0P

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(bicyclic oligopeptides as glucagon receptor inhibitors in relation to disease treatment and combination with other agents and metabolic stability)

IT 647807-36-1P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(bicyclic oligopeptides as glucagon receptor inhibitors in relation to disease treatment and combination with other agents and metabolic stability)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:60532 CAPLUS

DOCUMENT NUMBER: 140:105297

TITLE: Bicyclic oligopeptides and their use as glucagon receptor antagonists

INVENTOR(S): Potterat, Olivier; Streicher, Ruediger; Wagner, Klaus; Maurer, Till; Mack, Juergen; Peters, Stefan

PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. KG, Germany

SOURCE: PCT Int. Appl., 25 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004007524	A2	20040122	WO 2003-EP7311	20030708
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2004072736	A1	20040415	US 2003-621272	20030717
PRIORITY APPLN. INFO.:			EP 2002-15907	A 20020717
			US 2002-416797P	P 20021008

OTHER SOURCE(S): MARPAT 140:105297

ED Entered STN: 26 Jan 2004

AB The invention relates to a bicyclic oligopeptide or ester thereof having the capability to inhibit the glucagon receptor, which essentially consists of (a) a first cyclic group, which comprises at least one cysteine group and is formed by an amide bonding of the N-terminal amino acid with the second carboxylate group of a diacid amino acid, and (b) a second cyclic group which is formed by an amide bonding of an amino acid with the -carboxylate group of said diacid amino acid, and by a disulfide bonding of the C-terminal cysteine and a cysteine group within the first cyclic group (a); and to the use of such bicyclic oligopeptides for the

preparation of a medicament for the treatment or prevention of diseases, in which glucagon receptors are involved.

IT 647807-35-0P

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

(bicyclic oligopeptides as glucagon receptor inhibitors in relation to disease treatment and combination with other agents and metabolic stability)

IT 647807-36-1P

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(bicyclic oligopeptides as glucagon receptor inhibitors in relation to disease treatment and combination with other agents and metabolic stability)

L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:625549 CAPLUS

DOCUMENT NUMBER: 141:310378

TITLE: BI-32169, a bicyclic 19-peptide with strong glucagon receptor antagonist activity from *Streptomyces* sp
AUTHOR(S): Potterat, Olivier; Wagner, Klaus; Gemmecker, Gerd; Mack, Juergen; Puder, Carsten; Vettermann, Regine; Streicher, Ruediger

CORPORATE SOURCE: Boehringer Ingelheim Pharma GmbH Co. KG, Biberach an der Riss, D-88397, Germany

SOURCE: Journal of Natural Products (2004), 67(9), 1528-1531
CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 05 Aug 2004

AB A new bicyclic 19-peptide, BI-32169, was isolated from the culture broth of *Streptomyces* sp. (DSM 14996). Its structure was established by amino acid anal., mass spectrometry, and 2D NMR anal. BI-32169 consists exclusively of protein amino acids and is cyclized from the side chain of Asp9 to the N-terminus of Gly1. One disulfide bond between Cys6 and Cys19 forms a bicyclic structure. BI-32169 and its Me ester derivative showed potent inhibitory activity against the human glucagon receptor (IC50 440 and 320 nM, resp.) in a functional cell-based assay.

IT 647807-35-0P, BI 32169

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

(BI-32169 is a bicyclic 19-peptide from *Streptomyces* sp. with strong glucagon receptor antagonist activity)

IT 647807-36-1P

RL: BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(BI-32169 is a bicyclic 19-peptide from *Streptomyces* sp. with strong glucagon receptor antagonist activity)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L9 ANSWER 4 OF 4 USPATFULL on STN

ACCESSION NUMBER: 2004:95282 USPATFULL

TITLE: Bicyclic oligopeptides

INVENTOR(S): Potterat, Olivier, Mittelbiberach, GERMANY, FEDERAL
REPUBLIC OF
Streicher, Ruediger, Biberach, GERMANY, FEDERAL
REPUBLIC OF
Wagner, Klaus, Warthausen, GERMANY, FEDERAL REPUBLIC OF
Maurer, Till, Oberstadion, GERMANY, FEDERAL REPUBLIC OF
Mack, Juergen, Biberach, GERMANY, FEDERAL REPUBLIC OF
Peters, Stefan, Biberach, GERMANY, FEDERAL REPUBLIC OF
PATENT ASSIGNEE(S): Boehringer Ingelheim Pharma GmbH & Co. KG, Ingelheim,
GERMANY, FEDERAL REPUBLIC OF, 55216 (non-U.S.
corporation)

	NUMBER	KIND	DATE
PATENT INFORMATION:	US 2004072736	A1	20040415
APPLICATION INFO.:	US 2003-621272	A1	20030717 (10)

	NUMBER	DATE
PRIORITY INFORMATION:	US 2002-416797P	20021008 (60)
DOCUMENT TYPE:	Utility	
FILE SEGMENT:	APPLICATION	
LEGAL REPRESENTATIVE:	BOEHRINGER INGELHEIM CORPORATION, 900 RIDGEBURY ROAD, P. O. BOX 368, RIDGEFIELD, CT, 06877	
NUMBER OF CLAIMS:	17	
EXEMPLARY CLAIM:	1	
LINE COUNT:	732	

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB The invention relates to a bicyclic oligopeptide or ester thereof having the capability to inhibit the glucagon receptor, comprised of:

(a) a first cyclic group, which comprises at least one cysteine group and is formed by an amide bonding of the N-terminal amino acid with the second carboxylate group of a diacid amino acid, and

(b) a second cyclic group which is formed by an amide bonding of an amino acid with the α -carboxylate group of said diacid amino acid, and by a disulfide bonding of the C-terminal cysteine and a cysteine group within the first cyclic group (a); and

to the use of such bicyclic oligopeptides for the preparation of a medicament for the treatment or prevention of diseases, in which glucagon receptors are involved.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 647807-35-0P

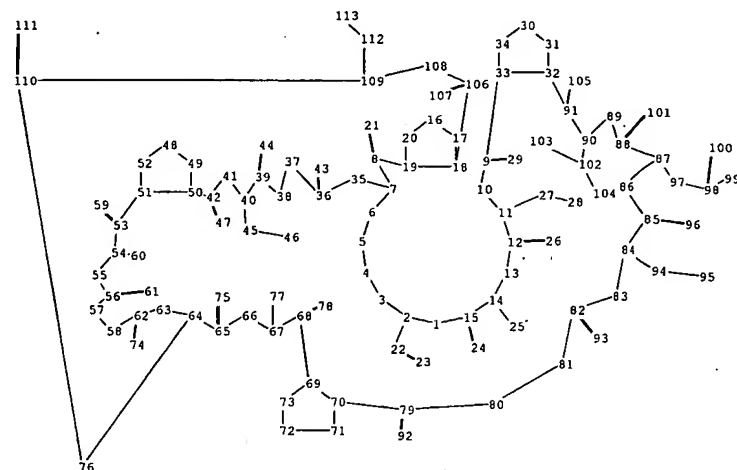
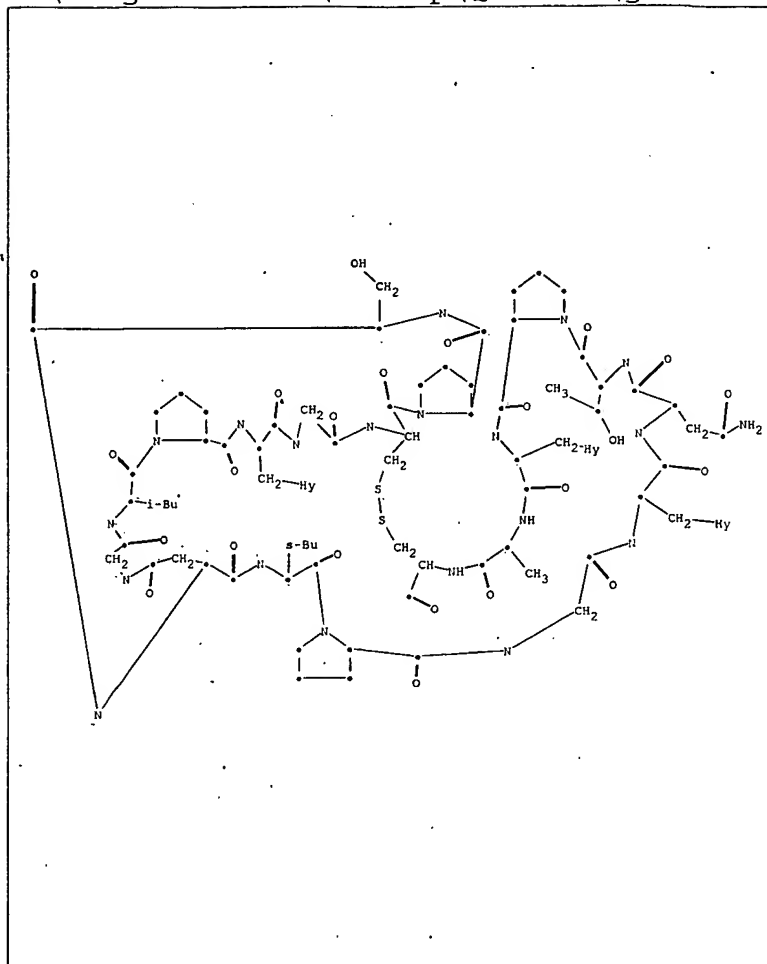
(bicyclic oligopeptides as glucagon receptor inhibitors in relation to disease treatment and combination with other agents and metabolic stability)

IT 647807-36-1P

(bicyclic oligopeptides as glucagon receptor inhibitors in relation to disease treatment and combination with other agents and metabolic stability)

FILE 'HOME' ENTERED AT 16:55:28 ON 05 DEC 2005

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chain nodes :

21 22 23 24 25 26 27 28 29 43 44 45 46 47 59 60 61 74
 75 77 78 92 93 94 95 96 97 98 99 100 101 102 103 104 105
 107 111 112 113

ring nodes :

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 31 32 33 34 35 36 37 38 39 40 41 42 48 49 50 51 52 53
 54 55 56 57 58 62 63 64 65 66 67 68 69 70 71 72 73 76
 79 80 81 82 83 84 85 86 87 88 89 90 91 106 108 109 110

chain bonds :

2-22 8-21 9-29 11-27 12-26 14-25 15-24 22-23 27-28 36-43 39-44
 40-45 42-47 45-46 53-59 54-60 56-61 62-74 65-75 67-77 68-78
 79-92 82-93 84-94 85-96 87-97 88-101 90-102 91-105 94-95 97-98
 98-99 98-100 102-103 102-104 106-107 109-112 110-111 112-113

ring bonds :

1-2 1-15 2-3 3-4 4-5 5-6 6-7 7-8 7-35 8-19 9-10 9-33 10-11
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 88-89 89-90 90-91 106-108 108-109 109-110

exact/norm bonds :

1-2 1-15 2-3 3-4 4-5 5-6 6-7 7-8 7-35 8-19 8-21 9-10 9-29
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 17-18 18-19 18-106 19-20 22-23 27-28 30-31 30-34 31-32 32-33
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53-54	53-59	54-55	55-56	56-57	56-61	57-58	58-62	62-63	62-74
63-64	64-65	64-76	65-66	65-75	66-67	67-68	68-69	68-78	69-70
69-73	70-71	70-79	71-72	72-73	76-110	79-80	79-92	80-81	81-82
82-83	82-93	83-84	84-85	85-86	85-96	86-87	87-88	88-89	88-101
89-90	90-91	91-105	94-95	98-99	98-100	102-104	106-107	106-108	
108-109	109-110	110-111							

exact bonds :

2-22	11-27	14-25	40-45	54-60	67-77	84-94	87-97	90-102	97-98
102-103	109-112	112-113							

Match level :

1:Atom	2:Atom	3:Atom	4:Atom	5:Atom	6:Atom	7:Atom	8:Atom	9:Atom	
10:Atom	11:Atom	12:Atom	13:Atom	14:Atom	15:Atom	16:Atom	17:Atom		
18:Atom	19:Atom	20:Atom	21:CLASS	22:CLASS	23:CLASS	24:CLASS			
25:CLASS	26:CLASS	27:CLASS	28:Atom	29:CLASS	30:Atom	31:Atom			
32:Atom	33:Atom	34:Atom	35:Atom	36:Atom	37:Atom	38:Atom	39:Atom		
40:Atom	41:Atom	42:Atom	43:CLASS	44:CLASS	45:CLASS	46:Atom			
47:CLASS	48:Atom	49:Atom	50:Atom	51:Atom	52:Atom	53:Atom	54:Atom		
55:Atom	56:Atom	57:Atom	58:Atom	59:CLASS	60:CLASS	61:CLASS	62:Atom		
63:Atom	64:Atom	65:Atom	66:Atom	67:Atom	68:Atom	69:Atom	70:Atom		
71:Atom	72:Atom	73:Atom	74:CLASS	75:CLASS	76:Atom	77:CLASS			
78:CLASS	79:Atom	80:Atom	81:Atom	82:Atom	83:Atom	84:Atom	85:Atom		
86:Atom	87:Atom	88:Atom	89:Atom	90:Atom	91:Atom	92:CLASS	93:CLASS		
94:CLASS	95:Atom	96:CLASS	97:CLASS	98:CLASS	99:CLASS	100:CLASS			
101:CLASS	102:CLASS	103:CLASS	104:CLASS	105:CLASS	106:Atom				
107:CLASS	108:Atom	109:Atom	110:Atom	111:CLASS	112:CLASS	113:CLASS			

Generic attributes :

28:	
Saturation	: Unsaturated
Number of Carbon Atoms	: 7 or more
Number of Hetero Atoms	: less than 2
Type of Ring System	: Polycyclic
46:	
Saturation	: Unsaturated
Number of Carbon Atoms	: 7 or more
Number of Hetero Atoms	: less than 2
Type of Ring System	: Polycyclic
95:	
Saturation	: Unsaturated
Number of Carbon Atoms	: 7 or more
Number of Hetero Atoms	: less than 2
Type of Ring System	: Polycyclic

=> fil reg; d que l10

FILE 'REGISTRY' ENTERED AT 17:03:29 ON 05 DEC 2005

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STRUCTURE FILE UPDATES: 30 NOV 2005 HIGHEST RN 869059-01-8

DICTIONARY FILE UPDATES: 30 NOV 2005 HIGHEST RN 869059-01-8

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TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

REGISTRY includes numerically searchable data for experimental and predicted properties as well as tags indicating availability of experimental property data in the original document. For information on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

sequence search

L10 2 SEA FILE=REGISTRY ABB=ON GLPWGCPDIPGWNTPWAC(SQSFP)

*family search
allows for conservative
substitution*

=> d sqide l10 1-2

L10 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN

RN 647807-36-1 REGISTRY

CN L-Cysteine, glycyl-L-leucyl-L-prolyl-L-tryptophylglycyl-L-cysteiny-L-prolyl-L-seryl-L- α -aspartyl-L-isoleucyl-L-prolylglycyl-L-tryptophyl-L-asparaginy-L-threonyl-L-prolyl-L-tryptophyl-L-alanyl-, 19-methyl ester, (9 \rightarrow 1)-lactam, cyclic (6 \rightarrow 19)-disulfide (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

SQL 19

NTE modified (modifications unspecified)

type	location	description
bridge	Gly-1 - Asp-9	lactam
bridge	Cys-6 - Cys-19	disulfide bridge

SEQ 1 GLPWGCPSDI PGWNTPWAC

=====

HITS AT: 1-19

****RELATED SEQUENCES AVAILABLE WITH SEQLINK****

MF C96 H127 N23 O24 S2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PRP (Properties)

****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

L10 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2005 ACS on STN

RN 647807-35-0 REGISTRY

CN L-Cysteine, glycyl-L-leucyl-L-prolyl-L-tryptophylglycyl-L-cysteinyl-L-prolyl-L-seryl-L- α -aspartyl-L-isoleucyl-L-prolylglycyl-L-tryptophyl-L-asparaginyl-L-threonyl-L-prolyl-L-tryptophyl-L-alanyl-, (9 \rightarrow 1)-lactam, cyclic (6 \rightarrow 19)-disulfide (9CI) (CA INDEX NAME)

OTHER NAMES:

CN BI 32169

FS PROTEIN SEQUENCE; STEREOSEARCH

SQL 19

NTE

type	location	description
bridge	Gly-1 - Asp-9	lactam
bridge	Cys-6 - Cys-19	disulfide bridge

SEQ 1 GLPWGCPSDI PGWNTPWAC

=====

HITS AT: 1-19

****RELATED SEQUENCES AVAILABLE WITH SEQLINK****

MF C95 H125 N23 O24 S2

SR CA

LC STN Files: CA, CAPLUS, USPATFULL

DT.CA Caplus document type: Journal; Patent

RL.P Roles from patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); USES (Uses)

RL.NP Roles from non-patents: BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PRP (Properties)

****PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT****

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

FILE 'CAPLUS, USPATFULL' ENTERED AT 17:05:29 ON 05 DEC 2005

=> s l10

L11 4 L10

=> s l11 not l8

L12 0 L11 NOT L8

=>

*printed
with structure
search*

*sequence search
yielded same 2
Registry records &
4 references that
the structure search
retrieved*

The ORTEP diagram illustrates the molecular structure of 2,2,4,4-tetramethyl-5-oxo-1,2,3,4-tetrahydropyridine-6-carboxamide. The molecule is shown as a solid model, with its symmetry-related counterparts (indicated by dashed lines) also visible. The structure features a central pyridine ring substituted with a carboxamide group and a 2,2,4,4-tetramethyl-5-oxo group. The diagram includes labels for atoms (C, N, O, S, H) and their corresponding displacement ellipsoid indices (e.g., 111, 110, 112, 108, 109, 107, 16, 17, 20, 21, 8, 19, 18, 9, 10, 11, 53, 50, 49, 48, 52, 51, 59, 41, 39, 40, 42, 43, 37, 38, 36, 35, 7, 6, 5, 46, 47, 45, 44, 43, 42, 41, 40, 39, 38, 37, 36, 35, 34, 33, 32, 31, 30, 29, 28, 27, 26, 25, 24, 23, 22, 21, 20, 19, 18, 17, 16, 15, 14, 13, 12, 11, 10, 9, 8, 7, 6, 5, 4, 3, 2, 1). The diagram also shows the presence of a water molecule (H₂O) and a disordered water molecule (H₂O) in the structure.

ORTEP diagram of the molecular structure of 2,2,4,4-tetramethyl-5-oxo-1,2,3,4-tetrahydropyridine-6-carboxylic acid. The structure shows a central pyridine ring with a carboxylic acid group at position 6 and a ketone group at position 5. The molecule is highly symmetric, with multiple equivalent positions indicated by numbers in parentheses. The diagram includes atom labels (C, N, O), bond lengths, and angles.

NODE ATTRIBUTES:

HCOUNT	IS	M1	AT	1
HCOUNT	IS	M1	AT	2
HCOUNT	IS	M2	AT	3
HCOUNT	IS	M2	AT	6
HCOUNT	IS	M1	AT	7
HCOUNT	IS	M1	AT	13
HCOUNT	IS	M3	AT	25

HCOUNT	IS M2	AT 27
HCOUNT	IS M2	AT 37
HCOUNT	IS M2	AT 45
HCOUNT	IS M2	AT 57
HCOUNT	IS M2	AT 60
HCOUNT	IS M2	AT 63
HCOUNT	IS M1	AT 77
HCOUNT	IS M2	AT 81
HCOUNT	IS M2	AT 94
HCOUNT	IS M2	AT 97
HCOUNT	IS M2	AT 99
HCOUNT	IS M3	AT 103
HCOUNT	IS M1	AT 104
HCOUNT	IS M2	AT 112
HCOUNT	IS M1	AT 113
HCOUNT	IS E1	AT 114
HCOUNT	IS E3	AT 115
HCOUNT	IS E3	AT 116
HCOUNT	IS E3	AT 117
HCOUNT	IS E2	AT 118
HCOUNT	IS E3	AT 119
NSPEC	IS R	AT 1
NSPEC	IS R	AT 2
NSPEC	IS R	AT 3
NSPEC	IS R	AT 4
NSPEC	IS R	AT 5
NSPEC	IS R	AT 6
NSPEC	IS R	AT 7
NSPEC	IS R	AT 8
NSPEC	IS R	AT 9
NSPEC	IS R	AT 10
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NSPEC	IS R	AT 16
NSPEC	IS R	AT 17
NSPEC	IS R	AT 18
NSPEC	IS R	AT 19
NSPEC	IS R	AT 20
NSPEC	IS C	AT 21
NSPEC	IS C	AT 22
NSPEC	IS C	AT 23
NSPEC	IS C	AT 24
NSPEC	IS C	AT 25
NSPEC	IS C	AT 26
NSPEC	IS C	AT 27
NSPEC	IS C	AT 28
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NSPEC	IS R	AT 40
NSPEC	IS R	AT 41
NSPEC	IS R	AT 42
NSPEC	IS C	AT 43
NSPEC	IS C	AT 44
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NSPEC	IS C	AT 46
NSPEC	IS C	AT 47
NSPEC	IS R	AT 48
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NSPEC	IS R	AT 58
NSPEC	IS C	AT 59
NSPEC	IS C	AT 60
NSPEC	IS C	AT 61
NSPEC	IS R	AT 62
NSPEC	IS R	AT 63
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NSPEC	IS R	AT 68
NSPEC	IS R	AT 69
NSPEC	IS R	AT 70
NSPEC	IS R	AT 71
NSPEC	IS R	AT 72
NSPEC	IS R	AT 73
NSPEC	IS C	AT 74
NSPEC	IS C	AT 75
NSPEC	IS R	AT 76
NSPEC	IS C	AT 77
NSPEC	IS C	AT 78
NSPEC	IS R	AT 79
NSPEC	IS R	AT 80
NSPEC	IS R	AT 81
NSPEC	IS R	AT 82
NSPEC	IS R	AT 83
NSPEC	IS R	AT 84
NSPEC	IS R	AT 85
NSPEC	IS R	AT 86
NSPEC	IS R	AT 87
NSPEC	IS R	AT 88
NSPEC	IS R	AT 89
NSPEC	IS R	AT 90
NSPEC	IS R	AT 91
NSPEC	IS C	AT 92
NSPEC	IS C	AT 93
NSPEC	IS C	AT 94
NSPEC	IS C	AT 95
NSPEC	IS C	AT 96
NSPEC	IS C	AT 97
NSPEC	IS C	AT 98
NSPEC	IS C	AT 99

NSPEC IS C AT 100
 NSPEC IS C AT 101
 NSPEC IS C AT 102
 NSPEC IS C AT 103
 NSPEC IS C AT 104
 NSPEC IS C AT 105
 NSPEC IS R AT 106
 NSPEC IS C AT 107
 NSPEC IS R AT 108
 NSPEC IS R AT 109
 NSPEC IS R AT 110
 NSPEC IS C AT 111
 NSPEC IS C AT 112
 NSPEC IS C AT 113
 NSPEC IS C AT 114
 NSPEC IS C AT 115
 NSPEC IS C AT 116
 NSPEC IS C AT 117
 NSPEC IS C AT 118
 NSPEC IS C AT 119

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 21 22 23 24 25 26 27 29 43 44 45 47 59 60 61 74 75
 77 78 92 93 94 96 97 98 99 100 101 102 103 104 105 107 111 112
 113 114 115 116 117 118 119

GGCAT IS PCY HIC LOQ UNS AT 28
 GGCAT IS PCY HIC LOQ UNS AT 46
 GGCAT IS PCY HIC LOQ UNS AT 95

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 119

STEREO ATTRIBUTES: NONE

L3 2 SEA FILE=REGISTRY SSS FUL L1

(FILE 'HOME' ENTERED AT 16:50:45 ON 05 DEC 2005)

FILE 'REGISTRY' ENTERED AT 16:50:53 ON 05 DEC 2005

L1 STRUCTURE UPLOADED
 L2 0 SEA SSS SAM L1
 L3 2 SEA SSS FUL L1
 SAVE TEMP L3 GUD272FULL/A
 D LC 1-2

FILE 'REGISTRY' ENTERED AT 16:52:21 ON 05 DEC 2005
 D QUE L3

FILE 'REGISTRY' ENTERED AT 16:52:58 ON 05 DEC 2005
 D STAT QUE L3

FILE 'CAPLUS, USPATFULL' ENTERED AT 16:52:58 ON 05 DEC 2005

L4 4 SEA ABB=ON L3
 L5 4 DUP REM L4 (0 DUPLICATES REMOVED)
 ANSWERS '1-3' FROM FILE CAPLUS
 ANSWER '4' FROM FILE USPATFULL
 D IBIB ED ABS HITSTR 1-4

FILE 'HOME' ENTERED AT 16:53:21 ON 05 DEC 2005

FILE 'REGISTRY' ENTERED AT 16:54:11 ON 05 DEC 2005

D STAT QUE L3

D IDE L3 1-2

FILE 'CAPLUS, USPATFULL' ENTERED AT 16:54:12 ON 05 DEC 2005

L6 4 SEA ABB=ON L3

L7 4 DUP REM L6 (0 DUPLICATES REMOVED)

ANSWERS '1-3' FROM FILE CAPLUS

ANSWER '4' FROM FILE USPATFULL

FILE 'REGISTRY' ENTERED AT 16:55:13 ON 05 DEC 2005

D STAT QUE L3

D SQIDE L3 1-2

FILE 'CAPLUS, USPATFULL' ENTERED AT 16:55:14 ON 05 DEC 2005

L8 4 SEA ABB=ON L3

L9 4 DUP REM L8 (0 DUPLICATES REMOVED)

ANSWERS '1-3' FROM FILE CAPLUS

ANSWER '4' FROM FILE USPATFULL

D IBIB ED ABS HITRN 1-4

FILE 'HOME' ENTERED AT 16:55:28 ON 05 DEC 2005

D QUE L3

FILE HOME

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STRUCTURE FILE UPDATES: 4 DEC 2005 HIGHEST RN 869277-23-6

DICTIONARY FILE UPDATES: 4 DEC 2005 HIGHEST RN 869277-23-6

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FILE LAST UPDATED: 4 Dec 2005 (20051204/ED)

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FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 1 Dec 2005 (20051201/PD)
FILE LAST UPDATED: 1 Dec 2005 (20051201/ED)
HIGHEST GRANTED PATENT NUMBER: US6971121
HIGHEST APPLICATION PUBLICATION NUMBER: US2005268363
CA INDEXING IS CURRENT THROUGH 1 Dec 2005 (20051201/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 1 Dec 2005 (20051201/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2005

```
>>> USPAT2 is now available. USPATFULL contains full text of the <<<
>>> original, i.e., the earliest published granted patents or <<<
>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<
```

```
>>> USPATFULL and USPAT2 can be accessed and searched together <<<
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<
>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<
```

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>

=> d his full

(FILE 'HOME' ENTERED AT 16:11:36 ON 02 DEC 2005)

FILE 'CAPLUS' ENTERED AT 16:11:55 ON 02 DEC 2005

```

                SET LINE 250
                SET DETAIL OFF
                E US2003-621272/AP, PRN 25
                SET NOTICE 1000 SEARCH
L1              2 SEA ABB=ON US2003-621272/AP
                SET NOTICE LOGIN SEARCH
                SET LINE LOGIN
                SET DETAIL LOGIN
                D SCAN
                SEL RN
    
```

FILE 'REGISTRY' ENTERED AT 16:12:43 ON 02 DEC 2005

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L2              26 SEA ABB=ON (10238-21-8/BI OR 105816-04-4/BI OR 111025-46-8/BI
                OR 122320-73-4/BI OR 135062-02-1/BI OR 141732-76-5/BI OR
                145375-43-5/BI OR 161600-01-7/BI OR 21187-98-4/BI OR 29094-61-9
                /BI OR 300865-11-6/BI OR 391208-93-8/BI OR 54249-88-6/BI OR
                56-03-1/BI OR 56180-94-0/BI OR 647807-35-0/BI OR 647807-36-1/BI
                OR 657-24-9/BI OR 72432-03-2/BI OR 89750-14-1/BI OR 9004-10-8/
                BI OR 9007-92-5/BI OR 9033-06-1/BI OR 93479-97-1/BI OR
                94-20-2/BI OR 97322-87-7/BI)
                D SCAN
L3              2 SEA ABB=ON L2 AND 19/SQL
                D SCAN
                D SQIDE
                E BRIDGE/NTE
                E LACTAM/NTE
                E DISULFIDE/NTE
                E CYCLIC/NTE
L4              2 SEA ABB=ON GLPWGCPDIPGWNTPWAC/SQSFP
                SAVE TEMP L4 GUD272SEQ/A
L5              2 SEA ABB=ON L4 AND L3
    
```

FILE 'REGISTRY' ENTERED AT 16:16:59 ON 02 DEC 2005

```

                D QUE L4
                D SQIDE L4 1-2
    
```

FILE 'CAPLUS, USPATFULL' ENTERED AT 16:17:28 ON 02 DEC 2005

```

L6              4 SEA ABB=ON L4
                D SAVED
    
```

FILE HOME

FILE CAPLUS

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FILE REGISTRY

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STRUCTURE FILE UPDATES: 30 NOV 2005 HIGHEST RN 869059-01-8
DICTIONARY FILE UPDATES: 30 NOV 2005 HIGHEST RN 869059-01-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

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```
*****
*
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*
*****
```

Structure search iteration limits have been increased. See HELP SLIMITS
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REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/ONLINE/UG/regprops.html>

FILE USPATFULL

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 1 Dec 2005 (20051201/PD)
FILE LAST UPDATED: 1 Dec 2005 (20051201/ED)
HIGHEST GRANTED PATENT NUMBER: US6971121
HIGHEST APPLICATION PUBLICATION NUMBER: US2005268363
CA INDEXING IS CURRENT THROUGH 1 Dec 2005 (20051201/UPCA)
ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 1 Dec 2005 (20051201/PD)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Oct 2005
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Oct 2005

```
>>> USPAT2 is now available. USPATFULL contains full text of the <<<
>>> original, i.e., the earliest published granted patents or <<<
>>> applications. USPAT2 contains full text of the latest US <<<
>>> publications, starting in 2001, for the inventions covered in <<<
>>> USPATFULL. A USPATFULL record contains not only the original <<<
>>> published document but also a list of any subsequent <<<
>>> publications. The publication number, patent kind code, and <<<
>>> publication date for all the US publications for an invention <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL <<<
```

>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc. <<<

>>> USPATFULL and USPAT2 can be accessed and searched together <<<
>>> through the new cluster USPATALL. Type FILE USPATALL to <<<
>>> enter this cluster. <<<

>>> <<<
>>> Use USPATALL when searching terms such as patent assignees, <<<
>>> classifications, or claims, that may potentially change from <<<
>>> the earliest to the latest publication. <<<

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substance identification.

=>